

# Detection of avoided crossings by fidelity

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The fidelity, defined as overlap of eigenstates of two slightly different Hamiltonians, is proposed as an efficient detector of avoided crossings in the energy spectrum. This new application of fidelity is motivated for model systems, and its value for analyzing complex quantum spectra is underlined by applying it to a random matrix model and a tilted Bose–Hubbard system.

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*Introduction.* – The enormous progress in cooling and manipulating ultracold atomic gases in recent years has opened new perspectives on interacting many-body models from condensed matter physics [1]. It led to questions and opportunities beyond conventional solid-state physics, e.g., the direct experimental study of quantum phase transitions [1], the role and engineering of genuine quantum correlations in such systems [1], and the phenomenon of quantum chaos in systems that consist of indistinguishable particles which lack an obvious classical counterpart [2–6]. In this context, it is possible to detect a quantum phase transition by the change of fidelity (modulus of the overlap between eigenstates of slightly different Hamiltonians) [7], since the ground state of a quantum system changes dramatically at a critical parameter [8].

Up to now, the temporal change of fidelity – as the overlap of the same initial states evolved by different Hamiltonians [9] – has been measured experimentally in wave billiards [10], but also in systems of cold atoms subject to optical potentials [11, 12]. Similar techniques may be applied to measure the evolving overlap of two eigenstates where time is substituted by the change of some tunable control parameter. Often a quantum phase transition may be viewed, for finite-size realizations of a system, as an avoided crossing (AC) in parameter space which closes in the thermodynamic limit [8]. A scenario of *many* ACs with a broad distribution of widths [13–15], as a manifestation of a strong coupling of many energy levels, is naturally found in quantum chaotic systems [13]. The question arises whether the applicability of fidelity can be lifted from pure ground-state analysis [16] to detect and characterize ACs in the entire spectrum of a complex quantum system. We show in this Rapid Communication that the fidelity indeed is a practically useful measure, which is local in the spectrum (detecting ACs of a single level) and connects changes in the wave function to parametric spectral dynamics.

*Fidelity measure.* – Given some parameter depending Hamiltonian  $H(\lambda) = H_1 + \lambda H_2$ , the fidelity [9] between the  $n$ -th eigenstates, denoted by  $|n\rangle$ , of slightly different Hamiltonians  $H(\lambda)$  and  $H(\lambda + \delta\lambda)$  is denoted as

$$f_n(\lambda, \delta\lambda) \equiv |\langle n(\lambda) | n(\lambda + \delta\lambda) \rangle|. \quad (1)$$

In complex quantum systems with many degrees of free-

dom, many of the levels of the system are coupled to each other leading to ACs in the spectrum of the Hamiltonian when the parameter  $\lambda$  is changed [13]. To simplify the discussion, we assume a finite size Hilbert space  $\mathcal{H}$ , where all energy levels are never exactly degenerate. To detect and characterize an AC for a given quantum level  $n$  we study the fidelity change [7]

$$S_n(\lambda, \delta\lambda) \equiv \frac{1 - f_n(\lambda, \delta\lambda)}{(\delta\lambda)^2} \quad (2)$$

which measures the change of the state  $|n\rangle$ . For  $\delta\lambda \ll 1$ , it is independent of  $\delta\lambda$ , i.e.  $S_n(\lambda, \delta\lambda) \approx S_n(\lambda)$ , and vanishingly small everywhere except in the vicinity of an AC. This fidelity measure also has the advantage of being applicable locally in the spectrum, where one follows a certain state  $|n(\lambda)\rangle$  and its neighbors over a range of parameter values  $\lambda$  to study the ACs they encounter. In addition, it is well-suited for numerical computations, since  $\lambda$  is the only relevant parameter as long as  $\delta\lambda$  is sufficiently small. The different limit of large  $\delta\lambda$  and hence the coupling over a broad energy band was the focus of a recent work using another generalized fidelity [17]. In contrast, our interest here is the detection and characterization of ACs as local couplings in energy space.

Let us first discuss two example systems. An isolated AC can locally be described in nearly-degenerate perturbation theory as an effective two-level system. It is then represented by a Hamiltonian  $H(\lambda) = \lambda\sigma_z + g\sigma_x$ , with a real coupling  $g$  between the levels ( $\sigma_x$  and  $\sigma_z$  denote Pauli matrices), showing an AC at  $\lambda = 0$  of width  $c = 2g$ . The normalized eigenstates are easily found [13] and the fidelity change in the limit  $\delta\lambda \ll 1$  can be computed exactly:

$$S_{1,2}(\lambda) = \frac{1}{8} \left( \frac{g}{g^2 + \lambda^2} \right)^2. \quad (3)$$

This is the square of a Lorentzian and differs significantly from zero only near the AC at  $\lambda = 0$ . This simple analytic formula allows us a better understanding of isolated ACs, as, for example, the peak width is easily computed as  $\sigma^{\text{FWHM}} = 2g\sqrt{\sqrt{2}-1}$ . On the other hand an AC can be characterized by the ratio between the local energy level curvature and the distance between the two repelling energy levels. We call the absolute value of this

ratio *renormalized curvature*  $C_n(\lambda)$  and find

$$C_{\pm}(\lambda) \equiv \left| \frac{1}{\Delta(\lambda)} \frac{\partial^2 E_{\pm}(\lambda)}{\partial \lambda^2} \right| = 4S_{\pm}(\lambda) \quad (4)$$

for the two-level system. For higher-dimensional systems we expand the wave function  $|n(\lambda + \delta\lambda)\rangle$  in second order in  $\delta\lambda$  and find

$$S_n(\lambda) = \frac{1}{2} \sum_{m \neq n} \frac{|\langle m(\lambda) | H_2 | n(\lambda) \rangle|^2}{[E_n - E_m]^2} \approx \frac{|\langle n'(\lambda) | H_2 | n(\lambda) \rangle|^2}{2[E_n - E_{n'}]^2},$$

where we reduced the sum near an isolated AC to the nearest neighboring level  $n'$ . Similarly, one obtains for the renormalized curvature [18]

$$C_n(\lambda) = \left| \frac{2}{\Delta(\lambda)} \sum_{m \neq n} \frac{|\langle m(\lambda) | H_2 | n(\lambda) \rangle|^2}{E_n - E_m} \right| \approx 2 \frac{|\langle n'(\lambda) | H_2 | n(\lambda) \rangle|^2}{[E_n - E_{n'}]^2} = 4S_n(\lambda). \quad (5)$$

The relation  $C_n \approx 4S_n$  thus holds as long as the effect of other levels can be neglected close to a single AC.

For very dense spectra and coupling between many levels, different ACs may lie close to each other. Three crossing levels can be generated, e.g., by the following real symmetric Hamiltonian

$$H(\lambda) = \begin{pmatrix} -\lambda & a & b \\ a & 0 & c \\ b & c & \lambda \end{pmatrix}, \quad (6)$$

which generalizes the above  $2 \times 2$ -model and contains already features of more complex systems. Fig. 1 shows that the fidelity change, defined in Eq. (2), is able to detect and to distinguish two nearby ACs in this system. Furthermore it resembles specific features of an AC in the shape of its peak, i.e., depending on the coupling  $g$ ,  $S_n(\lambda)$  shows a narrow peak of height  $S(\lambda = 0) = 1/(8g^2)$ . We see already in this simple example that the renormalized curvature captures the form of the fidelity change  $S_n(\lambda)$  close to an AC, with deviations arising from the admixture of a further level, which first and foremost effects the local curvature, i.e., the numerator in Eq. (4). But it also demonstrates that the fidelity change  $S(\lambda)$  itself is still effective in detecting and characterizing the ACs. *Application to complex systems.* – A highly dense spectrum with many and possibly overlapping avoided crossings is encountered in quantum chaotic systems as described by Random Matrix Theory (RMT) [13]. A prime example having such a dense complex spectrum is the combination of two random matrices drawn from the Gaussian orthogonal ensemble (GOE) [13]

$$H(\lambda) = \cos(\lambda)H_1 + \sin(\lambda)H_2, \quad H_1, H_2 \in \text{GOE}. \quad (7)$$

The distribution of minimal distances  $c$  at the ACs (normalized to unit mean) is then given by a Gaussian distribution  $P(c) = (2/\pi) \exp[-c^2/\pi]$  [14]. Using our fidelity

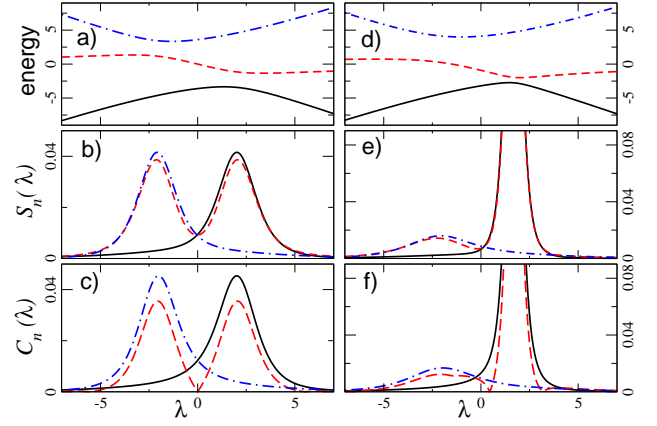


FIG. 1: (color online) (a) Energy spectrum of Eq. (6) for  $a = 0, b = 2, c = 3$ . All levels are coupled and the spectrum shows two close ACs; (b) fidelity change  $S_n(\lambda)$  and (c) renormalized curvature  $C_n(\lambda)$  for the energy levels of (a). (d) Energy spectrum for  $a = 1, b = 2, c = 3$ . All three levels are now directly coupled and the spectrum shows two close ACs. (e)  $S_n(\lambda)$  and (f)  $C_n(\lambda)$  for the energy levels of (d).

measure, we can directly detect the avoided crossings in this system and estimate also their widths. In the vicinity of a local maximum, the  $S$ -function has a Lorentzian shape as in Eq. (3) even in very dense quantum chaotic spectra. Under this assumption, we can thus extract the width of the AC as  $c = 2g = \sqrt{2S_{\max}}$ , c.f. Eq. (3), from the local maximum  $S_{\max}$ . Averaging over many ACs, the fidelity allows the verification of the RMT prediction with high accuracy. This is demonstrated in Fig. 2 for large random matrices.

To further exemplify the value of our fidelity measure, we apply it to a one-dimensional Bose-Hubbard Hamiltonian with additional Stark force [4, 6]. This example of a many-body Wannier-Stark system can be realized with ultracold atoms in optical lattices and the relevant parameters may be changed using well-known experimental techniques [1]. This model describes  $N$  particles on  $L$  lattice sites, with hopping between adjacent sites and a local on-site interaction. As exemplified in [4, 6], a gauge transformation into the force accelerated frame of reference turns a constant Stark force into a time-dependent phase  $\exp(\pm iFt)$  with periodicity  $T_B = 2\pi/F$  (the Bloch period). The corresponding Hamiltonian reads

$$H(t) = -\frac{J}{2} \sum_{l=1}^L (e^{iFt} a_{l+1}^\dagger a_l + \text{h.c.}) + \frac{U}{2} \sum_{l=1}^L n_l(n_l - 1), \quad (8)$$

where  $a_l^\dagger$  ( $a_l$ ) creates (annihilates) a boson at site  $l$  and  $n_l = a_l^\dagger a_l$  is the number of bosons at site  $l$ . The parameter  $J$  is the hopping matrix element,  $U$  the interaction energy for two atoms occupying the same site, and  $F$  the Stark force. Periodic boundary conditions are imposed for  $H(t)$ , such that the Hamiltonian and the one-period Floquet operator  $\hat{U}_F(T_B) =$

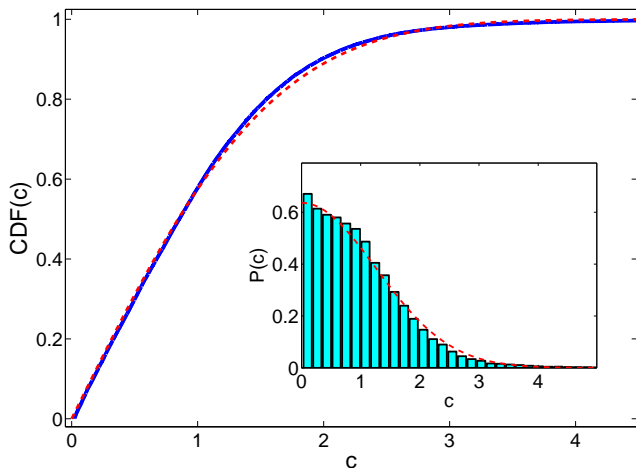


FIG. 2: (color online) Cumulative distribution of ACs determined from the fidelity change maxima for the RMT model of Eq. (7) with  $\dim H_{1,2} = 1024$  and  $\lambda \in [0, \pi[$  showing ca. 30,000 ACs: the numerical distribution (solid line) in excellent agreement with the RMT prediction  $CDF(c) = \text{erf}(c/\sqrt{\pi})$  (dashed line). *Inset*: Distribution of widths of the ACs  $P(c)$  (histogram) and the RMT prediction (dashed line).

$\mathcal{T} \exp \left( -i \int_0^{T_B} H(t) dt \right)$  (where  $\mathcal{T}$  denotes time-ordering) decompose into a sum of operators for specific quasimomenta  $\kappa$  [4]. In the following, we use  $F$  as a control parameter. For  $J \approx U \ll F$  the quasienergy spectrum (eigenphases of  $\hat{U}_F(T_B)$ ) is dominated by the force  $F$  and the system is regular. Decreasing the force to  $J \approx U \gtrsim F$  the quasienergy spectrum reorders and the coupling between the levels becomes more important. For fillings of order unity, e.g.  $N/L \approx 1$ , the system is quantum chaotic in this regime and the spectrum obeys Wigner-Dyson statistics [4, 6]. As  $F$  is varied one observes an increasing number of ACs as the spectrum is changing and additionally many broad ACs once the quantum chaotic region is reached.

To illustrate the crossover between regions with few and many ACs, we study the density of ACs as detected by the fidelity change  $S_n$ , when changing the system parameter  $\lambda$ . In a histogram, the density  $\rho_{AC}(\lambda)$  is defined via  $\rho_{AC}(\lambda) \cdot d\lambda = N_{AC}(\lambda)/\dim \mathcal{H}$ , comparing the number of ACs  $N_{AC}(\lambda)$  in the interval  $[\lambda, \lambda + d\lambda]$  to the total number of energy levels  $\dim \mathcal{H}$ . This is shown in the main part of Fig. 3 where we observe no ACs at large  $F$ , i.e., small values of  $1/F$ , and an increasing number of ACs for larger values of  $1/F$  that saturates around  $1/F \approx 20$ . The mentioned transition between regular and chaotic spectral properties for  $J \approx U$  and  $F \ll J$  and approximately integer filling in the tilted system can be visualized by comparing the actual level spacing distribution to a Wigner-Dyson distribution using a standard statistical  $\chi^2$  test [6]. This is displayed in the inset of Fig. 3 along with the density of ACs in Fig. 3. The fidelity change  $S(1/F)$  detects ACs and marks the crossover from regular

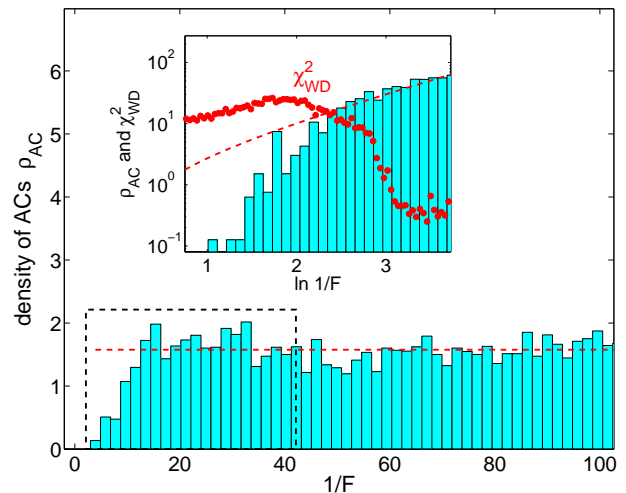


FIG. 3: (color online) Density of ACs  $\rho_{AC}$  in the quasienergy spectrum of the Floquet operator of our Bose-Hubbard model for varying  $F$  and fixed  $J = 0.038$ ,  $U = 0.032$ ,  $N = L = 6$ . The number of ACs as detected by the fidelity change increases with  $1/F$  and saturates around  $1/F \approx 20$  to an average value which is shown by the dashed line. *Inset*: Magnification of the region marked by the box on logarithmic scale with a comparison to a  $\chi^2$  test (with small values for good Wigner-Dyson statistics [6]).

to chaotic dynamics, showing the same qualitative behavior as the spectral statistics: in regions of good Wigner-Dyson statistics we find a high density of ACs compared to a smaller number of ACs in the regular regime. The crossover beginning for  $\log(1/F) \approx 2$ , where the density of ACs rises above unity, i.e., on average each energy level undergoes more than one AC in the unit interval. The transition is complete for  $\log(1/F) \approx 3$  where the  $\chi^2$  test saturates around a low value.

A clear advantage of the fidelity change compared to spectral statistics is that it can be applied *locally* in the spectrum. This means that, if one is interested only in local spectral properties of a system, it is sufficient to follow a small number of levels to characterize the system's behavior. On the other hand, it means if we follow all energy levels over a certain parameter range, we can resolve remarkable details in the full spectrum. This can be done easily by using the fidelity change in order to detect and characterize ACs. With this method we are, e.g., able to detect a small number of regular states [19] traversing the chaotic sea of energy levels in the chaotic regime of the tilted Bose-Hubbard model. In this case the distribution of widths of ACs is a mixture of regular and quantum chaotic distributions:

$$P(c) = (1 - \gamma)\delta(c) + \frac{2\gamma^2}{\pi c} \exp \left[ -\frac{\gamma^2 c^2}{\pi c^2} \right], \quad (9)$$

with a chaotic part of weight  $0 \leq \gamma \leq 1$  [20]. A finite regular component makes itself visible as a strong enhancement of  $P(c)$  close to zero, c.f., the inset of Fig. 4.

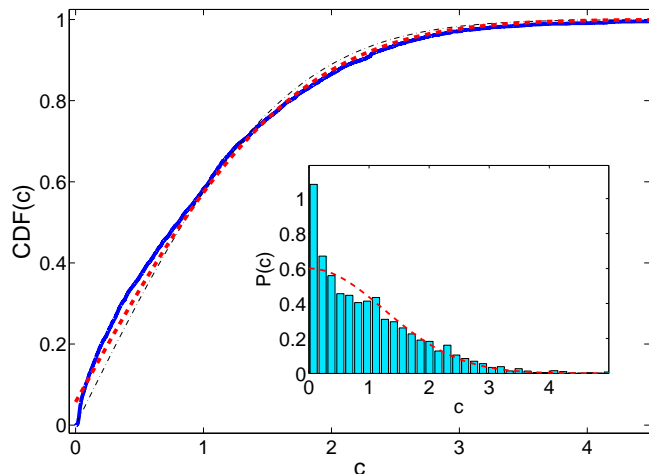


FIG. 4: (color online) Cumulative distribution of ACs determined from the fidelity change maxima for the system of Eq. (8). Shown are the numerical distribution (solid line), the best fit for a mixed RMT spectrum (thick dashed line, chaotic part  $\gamma \approx 0.94$ ), and the RMT prediction for a purely chaotic spectrum (thin dashed-dotted line). Parameters:  $N = 6, L = 7, J = 0.038, U = 0.032, F = 1/39 \dots 1/35$ . *Inset:* Distribution of widths of ACs for the same model (histogram) and Eq. (9) with  $\gamma \approx 0.94$  (dashed line). The enhancement peak close  $c = 0$  arises from the regular “solitonic” states [19] in the spectrum.

We are also able to estimate the size of this component by analyzing the cumulative distribution function  $CDF(c) = 1 - \gamma + \gamma \operatorname{erf}\left(\frac{\gamma c}{\sqrt{\pi}}\right)$ . The result is shown in the main part of Fig. 4, where we plot the numerically ob-

tained distribution and the best  $\chi^2$ -fit including a finite regular component. We obtain a chaotic part of  $\gamma \approx 0.94$ , corresponding to ca. 6% of regular levels, in good agreement with counting 7 regular levels out of 132 by direct inspection of the spectrum. Except for the identification of single regular levels [19], this has so far not been detected in the tilted Bose–Hubbard model by other statistical measures. The reported results are obtained for periodic boundary conditions applied to the Hamiltonian of Eq. (8), but we found a qualitatively similar picture for hard-wall boundary conditions, as used in [19]. Our results underline the value of fidelity as a measure for detecting ACs with high resolution in complex energy spectra.

*Summary.* – We showed that quantum fidelity is perfectly suited to detect and characterize ACs in the energy spectrum. It therefore connects information about the wave function of a system with its spectrum, without direct reference to the energy levels by using only the overlap of wave functions [21]. This has been exemplified for simple models and for complex quantum systems showing many ACs. The fidelity of Eq. (2) can be applied to characterize the system’s behavior locally in energy space, i.e., parts of spectrum only, as is the typical situation in experiments where the complete spectrum is not accessible in most cases. The fidelity, therefore, proves very useful to study many-body systems, also beyond their ground-state properties [7].

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